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Computational Fluid Dynamics Models of Molecularly Imprinted Materials in Microfluidic Channels

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ABSTRACT

Current research will lead to rapid-prototyping of chemical sensors that utilize microfabricated molecularly imprinted (MI) materials. CFD/CAD software may be used to model flow and chemical binding properties of MI materials in microfluidic channels. Use of this type of software expedites results when changes in properties are made. The surface concentration of bound analyte on a monolithic molecularly imprinted polymer (MIP) within microfluidic channels can be modeled using its experimental binding kinetics. The time necessary to reach a detection limit is calculated and optimized as a function of flow parameters. In this report, we discuss the unique issues associated with the modeling of chemical sensors that utilize MI materials.

INTRODUCTION

In the broadest sense, device engineering is a multi-step process that includes 1) design concept, 2) computer aided design (CAD) and computer aided modeling (CAM), and 3) prototype fabrication. The utilization of CAD/CAM allows the engineer to iteratively optimize a device design before prototype fabrication. Thus, CAD/CAM adds to the efficiency of the device engineering process. Presently, this paradigm has entered into the device engineering sub-discipline of microfluidic devices, often called 'lab-on-a-chip'. CAD/CAM software under development by several research groups and companies offer the capabilities to model fluid flow in micrometer-scale channels using computational fluid dynamics (CFD). Added capabilities include simultaneous modeling of fluid flow, chemical reactions, and analyte binding to surfaces. Our project is concerned with the incorporation of molecularly imprinted materials into this device engineering paradigm. We seek to determine the properties of MI materials which are most relevant to the ultimate performance of devices and thus to the device engineer. In this paper, we will focus on the CAD/CAM issues. We report our initial experience adapting available software along with a simple example that illustrates present design and modeling capabilities, and provide a list of properties that are necessary for designing with MI materials. Ultimately, this work points the way to the generation of a database of MI material properties incorporated into software for the engineer to use in new device designs. We hope our list will encourage the reporting of these properties as new MI materials are developed and optimized.

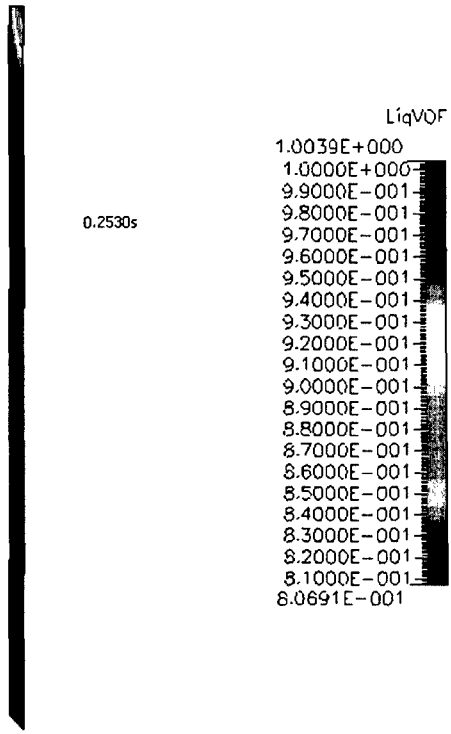

Figure 1: Flow model in a microfluidic channel.

COMPUTATION DETAILS

Materials properties of a recently reported MI polymer were used in the model we report here.[1]

The software used in the project was obtained from CFD Research Corporation, 215 Wynn Dr., Huntsville, AL 35805. This software contains 3 components: CFD-Geom where the geometric models can be drawn and gridded; CFD-ACE where analysis is done; and CFD-View to view by 2 and 3 dimensions and animation.

The CFD ACE+ software was used to demonstrate flow and binding in a microfluidic channel 100 microns in diameter.

A typical design drawing begins with wire frame models drawn in 2 or 3 dimensions. These are then gridded for finite element analysis .[2] We chose to start with a simple straight 2D microfluidic channel 100 microns wide. The volume is separated into three sections, to allow different properties in the center 'patch'. Flow is modeled first with the channel initially filled with water, then at t=0, flow begins with the analyte solution. This first model shows the channel nearly full of the analyte fluid at a t= 0.25 seconds at an initial velocity of 0.02 m/s (12µl/min), 0 pressure, and T=300K (Figure 1.).

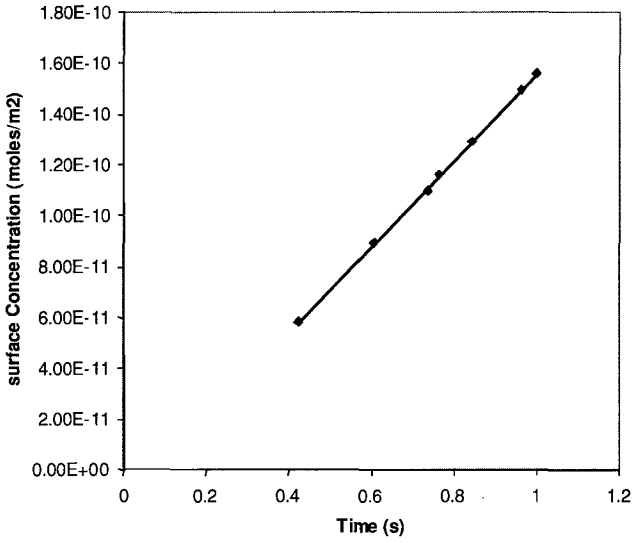

Figure 2. Time vs. Surface Concentration at an analyte concentration of $1x10^{-5}$M.

The next step introduces the values for binding kinetics (determined by experiment), and other variables. For instance:

Density of receptors= maximum possible surface concentration = $5x10^{-8}$ mole/m^2
Association rate constant = 41.2 $M^{-1}s^{-1}$
Disassociation rate constant = $3.21x10^{-4}$ s^{-1}

To show the changes in histamine binding on the surface over time, an analyte concentration of $4.5x10^{-8}$M was chosen and the surface concentration determined at 1.0, 4.9, 7.5, and 10.0 seconds. The results show that less than 4.9 seconds are needed to reach a steady state surface concentration of 10^{-13}M

To show velocity effects, all variables are kept the same except the inlet velocity. The inlet velocity was varied between 0.001m/s and 0.002 m/s to look at changes in the concentrations at the surface. Effects of changing the analyte concentration from 1M to $1x10^{-5}$M were also investigated.

The flow models show some time constraints of velocity changes. For instance, if the channel needed to fill in one second, a velocity greater than 0.02 m/s is required.

Using data from different times at the same analyte concentration it can be determine that it would take 5.1 seconds to have a detectable surface concentration based on a Mach-Zehnder interferometer (Figure 2).

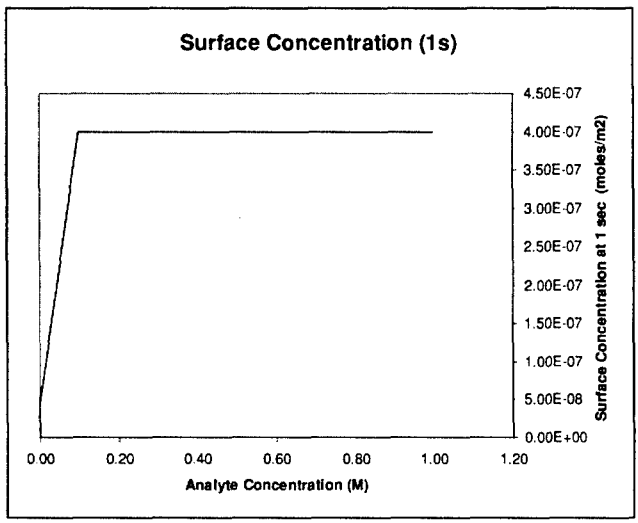

Figure 3. Analyte concentration vs. surface concentration at 1 second.

Investigating the surface concentration as the analyte concentration is changed, the limit of binding can be determined. This is based on the density of receptors possible ($5x10^{-8}$mole/m^2). At an analyte concentration of 1M, the maximum binding is reached at 1 second (Figure 3).

CONCLUSION

Computer modeling expedites the device engineering process when chemical and geometric changes are made. The simple example presented above demonstrates that fluid and MI material properties are critical for a complete and accurate design (Table 1). Furthermore, as new MI materials are developed, monomer formulation properties that may be needed by device fabrication methods should be considered also.[3] For example, low viscosity monomer formulations may be required for certain well-known techniques.[4] In another example, a materials' optical properties might dictate to the engineer the choice of an optical detector to use with a highly transparent imprinted acrylate. In conclusion, we hope that this paper will encourage dialog between the MI materials synthesis and the engineering communities during the early stages of MI material development for more efficient production of new devices that utilize MI materials.

Table 1. List of Important Kinetic and Materials Properties for CFD/CAM

Fluid	MI Material
viscosity	association rate constant
density	dissociation rate constant
velocity	irreversible rate constant
surface tension	diffusivity
analyte concentration	receptor density
elasticity	surface roughness

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